Transparency, Reproducibility and Quality of Energy System Analyses – a process to improve the scientific work

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Introduction

The general lack of transparency in energy system modelling leads to irreproducible results and the loss of traceability in decision making, which contradicts the general requirements for good scientific work. In 2012, the report of the EU-funded project *ATEsT* stated: "*increasing the transparency in supporting of the EU RD&D policy initiatives was suggested as an overall action.*" [ATEsT 2012]. Beside of leading to incomprehensible policy this lack of transparency is an important obstacle to the scientific debate on energy system modelling. A profound discussion about the strengths and weaknesses of the existing models and which questions can or cannot be answered by them is hampered. The *openmod initiative*[1] writes in their manifesto: "*We believe that more openness in energy modelling increases transparency and credibility, reduces wasteful double-work and improves overall quality.*" [openmod]. In an article [Pfenniger 2017] states for further specification of the problem: "*Sharing a DNA sequence in an established format is, of course, easier than sharing the unstructured assumptions behind a techno-economic scenario study, for which no standard format exists yet. So the energy community must decide on standards for sharing code, data and assumptions.*" This paper picks up the thread and aims to contribute to a standardisation process of sharing information about energy system analyses. Light is shed on the gap between opening up and reaching transparency or even reproducibility. The latter is defined according to the rules of the German Research Society (DFG) for good scientific practice. Transparency can thus be seen as a necessary precondition for reproducibility. Both transparency and reproducibility are just a part of the criteria for the quality of models or data. In the present paper the focus is set on transparency and reproducibility. The research is based on an in-house application that can be generalised. The main goal is to document the applicability of existing tools and open it up for further discussions. Some of the evaluated tools as well as the suggestions for improvement were designed through to cross-institutional collaboration and expert workshop which were a fundamental part of the on-going research projects *open_eGo [open_eGo]* and *open_FRED [open_FRED]*. The general framework outlined above leads to the following research questions that we want to address:

- What is the status-quo of transparency/reproducibility in the selected case study?
- Which areas need improvements?
- How can these improvements look like?

Methodology

At the outset, the necessity for a clear and intelligible definition of key terms is addressed. In contrast to the usually separate sections for abbreviations and definitions in each publication a collective public documentation was started. A shared glossary has the aim to develop a common understanding of terms. This way the different interpretations and applications become apparent and can be discussed openly. In addition to the definitions, supplementary

[1] open energy modelling initiative: an international grass root initiative of modellers from various organisations

information (abbreviations and sources) and relations (synonyms and subterms) augment the concept towards an ontology. A German equivalent can be found on the central information system EnArgus [BMWi]. Following this, the options to use different types of licenses for data, software and artwork are presented.
The main task is the application of a transparency checklist as it is described in [Cao 2016] to a case study and carry out a critical self-observation in order to develop, present and evaluate standardised tools. In addition to the published report, all accompanying materials that are publicly available are assessed critically. This comprises the compiled input data including assumptions, the created energy system model and, of course, the resulting data. The transparency assessment of the interpretation of the results as well as of the finding of conclusions is not part of this investigation (see Figure 1).

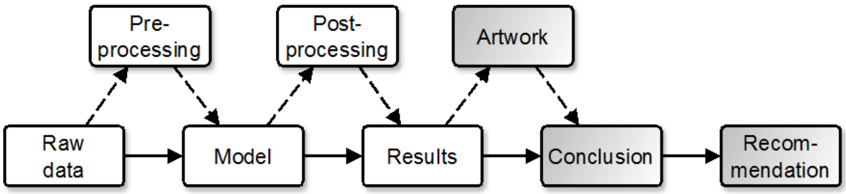

Figure 1: Simplified model flow. Figure by Ludwig Hülk / CC BY SA 4.0

The ideas, templates and tools developed in the above-named research projects are presented. These are the multi-level and linked “fact sheets”, the “OpenEnergy Database”(oedb) and the “scenario log”. Central idea of the factsheets is to provide a standard online form to simplify the input of information, to provide a clearly arranged representation and to facilitate the public availability. The developing process of the fact sheets included an evaluation of the transparency checklist, the list of open models from the [openmod-wiki] and other materials and contributions from different institutes. In two expert workshops and in online discussions the fact sheets have been improved and divided into fact sheets for frameworks, models, and scenarios.
The three kinds of factsheets were implemented as part of the OpenEnergy Platform - an in-progress component of the open_eGo project - and parts of it have also been added to the wiki of the openmod-initiative. The search and filter functionalities of model and framework factsheets yield huge improvements regarding inter-project communication and possible and intended code reuse.

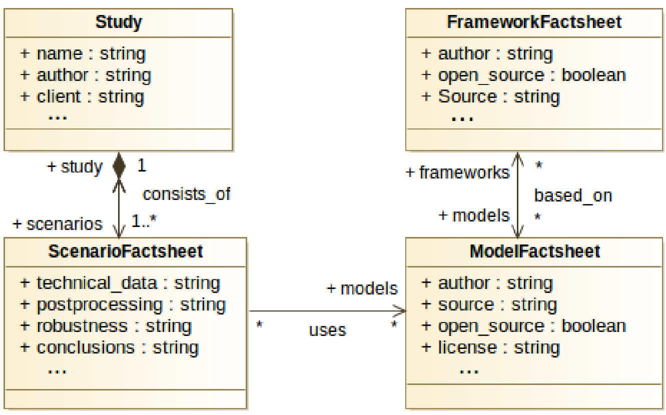

Figure 3: UML class diagram of fact sheets. Figure by Martin Glauer / CC BY SA 4.0

External developers get an overview on existing functionalities and methods which they can reuse with respect to the corresponding licenses. In this way double work is avoided, since typical functions used in energy system models do not need to be developed over and over again. Additionally, mistakes are eliminated, because different model developer and users

work with the code and can report bugs and help debugging. Users that are inexperienced and new in the field of energy modelling get a quick overview on existing frameworks and models that can be used for their purposes and immediate information on the data sets that might be used and publications addressing said tools.
Whilst model- and framework factsheets are rather technical and mostly interesting for programmers, scenario factsheets tackle some of the introductory mentioned flaws in current scientific energy modelling. The given meta information illuminates the necessary assumptions that lead to specific results. Scenario factsheets contain information not only on used data and models, but also on the parameter configuration they were used with. This yields the possibility to get an overview on scenarios that used similar assumptions, which might allow conclusions on the impact of specific parameters influencing the results of energy models.

The OpenEnergy Database will not play an important role in this paper. In the projects, it is used to exchange and publish data but there are different possibilities to give access to data. One strength of the oedb is to provide metadata which increases the quality of the data.
A supplementary method of documentation is presented that was developed to improve reproducibility. Comparable to a kind of logbook, the “scenario log” records work steps and data flows. The implemented functions aim at high automation while following the basic principles of good scientific practice; this can be seen as an adapted edition of the well-known laboratory notebook.
As case study, a current research assignment is selected, using a comparatively simple model and a reduced scenario frame. The regional association of the German green political party *Bündnis 90/Die Grünen* has commissioned a research study in order to assess the impact of the energy strategy 2030 [MWE 2012] of the federal state Brandenburg. The main focus was the investigation of changes in the political and economic conditions regarding lignite utilisation and the fulfillment of the CO_2 reduction targets. The approach was to build a model of the local energy system considering heat and electricity demand and generation. It is based on the *open energy modelling framework* (oemof) [oemof 2016] and is called *oemof app Berlin Brandenburg* (abbb). Different types of heat and power generation, the projected consumptions and the expected export of electrical energy are taken into account to determine load flows in and between the five subregions and the surrounding export regions on an hourly basis. In three scenarios carbon dioxide emissions, the utilisation of existing power plants as well as of the existing grid, have been analysed to examine the viability of the energy strategy. The final report aims at weighing up between a technical documentation, simple comprehension for non-experts, clear recommendations for action and maximal transparency.

Results

Though the glossary is not yet used very widely it provides a possibility to refer to public available definitions. All terms used in the fact sheets can be clarified there. Examples for terms with diverging definitions which have been discussed along the projects are “scenario”, “endogenous”- and “exogenous” parameters, “processed data” or “secondary data”.

One crucial point that appears when the data shall be opened up for common use is the question of licenses. Making data publicly available doesn’t mean automatically that it can be used. A license clarifies the conditions under which data or code can be used. In the absence of a license, the author retains proprietary copyright. Standard licenses provide pre-

defined sets of standard conditions. The most common licenses for a given artefact can be determined by its type: code, data, documentation or other generic digital "creative work" like figures and maps. For any given project, these components can and should be licensed independently by type. At the most basic level, one must decide on whether to use a copyleft license or a more permissive license. While copyleft assures that code changes by any future contributors must stay public, permissive licenses only require attribution in derived works.

The central tool applied in this study is the transparency checklist [Cao 2016]. It is structured into ‘General Information’, ‘Empirical Data’, ‘Assumptions’, ‘Modeling’, ‘Results’, and ‘Conclusions and Recommendations’. Evaluating the transparency checklist and applying it to a study lead to two additional sorts of categorisation of the questions. The development of standardised fact sheets resulted in the categorisation of framework-, model- and scenario factsheets to avoid redundant information. Furthermore a differentiation of the questions into “general transparency”-, “reproducibility”- and “quality”-related questions has been implemented. “General transparency” includes facts that are not necessary for reproducibility as e.g. name of author, licence, etc.. “Reproducibility” are those facts of transparency that are necessary to reproduce the work. Whereas “quality”-related questions are including those questions that are evaluating the quality of the study and are not related to transparency. Especially this differentiation seems important because making a model or scenario simulation transparent doesn’t mean that it’s quality is high, it just allows to evaluate the quality.
To apply the checklist to our study we used all documents and data that will be available after its publication including the report, the database tables and the fact sheets. The letter were the most important sources of information. Links to the material will be published on the [RLI-project-page].
The full list of questions with categorisation and the evaluation of our study can be found through to [checklist-categories]. Table 1 shows the results of the evaluation. The first column (“field”) comprises the original categories of the transparency checklist. The columns “T”, “R” and “Q” declare how many questions of this category have been assigned to transparency, reproducibility and quality respectively. The “Score”-columns show how many of the questions of this category could be answered with the publicly available information.

Table 1: Results of the application of the checklist per category

Field	T	Score	R	Score	Q	Score	Total
General Information	6	83%	0	-	2	100 %	88%
Empirical Data	0	-	2	100%	1	100 %	100%
Assumptions	3	100%	2	100%	6	33 %	64%
Model exercise	6	100%	5	80%	3	67 %	86%
Results	0	-	2	0%	2	50 %	25%
Conclusions and Recommendations	0	-	0	-	5	20 %	20%
sum / average	15	93%	11	73%	19	47 %	45 / 69%

The evaluation shows that only one question concerning general transparency (1.2 “What are the authors’ contributions in detail?”) couldn’t be answered. The development of the model code can be tracked in the version control of GitHub. Other parts like data processing and writing of the final report are not documented openly yet. Concerning the category

reproducibility, the score of 73% is also improvable. This is due to missing openness of the output data and post-processing (14.1 “Where can one find the numerical values (output) of the model?”). One possible solution is an import into the database. Quality-related questions are only partly answered. Most of these questions are addressing the issues assumptions, uncertainties and validation. This are important issues that can be answered in the documentation or the final report.
Concerning reproducibility, the transparency checklist is not yet sufficient. It is not evaluated if the used data is published and if the published data is clearly arranged. Furthermore the process of model implementation or linking models is not evaluated.

The modelling process is described with the following steps [openmod manifesto]: input of raw data - data processing - model formulation – numerical solver – model output – interpretation (see also figure 1). Opening it up means for the first two steps that "Open Data" is requested. For the processing as also for step three and four open source software (scripts, models, packages, etc.) is needed to open up. Step five is not a big challenge to open up as model results are usually published. The question is if all output data (before post-processing) should be included. We left step six "interpretation" for a future work. We would even see it as two steps "conclusions" and "recommendations" where the process and criteria should be defined and opened up.
Due to the heterogenous landscape of TSOs and other energy providers in europe as well as the decentralised structure of the scientific community, there is a vast amount of different data structures and sources. This raises the difficulty to agree upon a common basis to compare models. Hence, a common source of energy data that merges different data models into a usable and comparable structure is mandatory. The Open Energy Database[oedb] was developed to provide a place where raw data and processed data can be published and linked to. Using that for the simple scenario served the expectations though endogenous data will not be in the database but only in the model. Even if the model is also open source the used data cannot be found in one place which results in less transparency. This can be avoided by making endogenous data available in the model fact sheet. To really reference every used value can result in a very time consuming work if a number of single cells of a table have to be commented. The process foreseen for this in the oedb is still too complicated and needs automatisation.
To also open up the process of model implementation or even scenario simulations with linked models we developed the “scenario log”

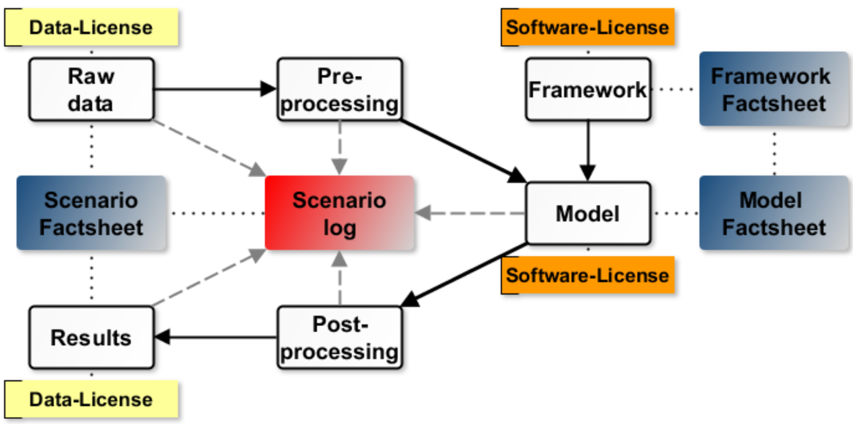

Figure 2: Enhanced model flow. Figure by Ludwig Hülk / CC BY SA 4.0

The scenario log is based on the idea of an analog laboratory notebook as organisational tool to record different kinds of actions from multiple users. In our case the implementation is

done in a simplified database table where entries are added each time a script or program is being executed (see grey arrows in Figure 2). From the perspective of the database and the data flow there are different possible actions like input and output. In addition to this, useful information can be added manually or is obtained automatically (*), see Table 2. While there are no standardised guidelines for documentation, one common criteria is the use of permanent entries. This is implemented by the user rights, which do not allow deletion or modification but only inserts.

Table 2: Description of the scenario log

Entry	Description	Example
id*	Serial number, unique identifier	1
version	Version number of programme or script	v0.1
action	Type of action or data flow	setup, import, export, input, output
path	Database or file path	schema.table
source	Name of the script or programme	egodp_rea_setup.sql
comment	Additional information	Setup script
user_name*	Name of the database user	exampe_user
timestamp*	Date and time	2017-02-17 16:20:00
metadata*	A copy of the metadata if available	{metastring}

Conclusion

Due to the evaluation of the status-quo of the transparency, we identified areas that need an improvement. The comparison of the checklist with the case study shows that the majority of the transparency (93%) and reproducibility (73%) criteria are fulfilled. Only the questions concerning the actual contributions of each author and the output data are not answered yet. The presented scenario log is one possible solution to record individual work steps and data flows in order to increase transparency. Missing output data can be imported into the OpenEnergy Database or can be published elsewhere online. Questions categorised as quality criteria are only answered partly (47%). Standardised solutions to answer the issues of documenting assumptions, uncertainties and validation must be developed in the future works. The analysis shows that the fact sheets are suitable to record the most important information and further provide other useful functions like predefined answers and filters.

New processes and instruments have been developed to improve transparency, reproducibility and thus the quality of energy system analyses. The overall concept of good scientific practice should include a variety of different tools and solutions. This should cover different areas from proper licensing to a complete publication of accompanying materials. This compilation is intended to be a further step towards a holistic view of the scientific work.

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